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NJOY2016 updates for ENDF/B-VIII.0

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Chapter 1

Introduction

Each release of the ENDF/B library often results in the introduction of new data formats in the ENDF-6 format. With ENDF/B-VIII.0 [1], which was released in February 2018, new formats were added for allowing tabulated fission energy release components in the MF1/MT458 section, to allow for sub-actinide fission and non-neutron induced fission in the MF8/MT18 and MF10/MT18 sections, and to add fission neutron and gamma emission probabilities in the MF6/MT18 section [2]. Processing codes must be adapted to ensure that they are capable of using these new data, or at the very least understand the new formats. NJOY2016, the production version of the nuclear data processing code developed at Los Alamos National Laboratory is no exception to this.

In addition to format changes, a new evaluated nuclear data library also tends to push the limits of the processing codes leading to a number of fixes and updates to correct problems that were uncovered while processing the beta releases and final release of ENDF/B-VIII.0:

- updates to ACER for plot generation and thermal scattering data formatting;
- updates to ERRORR for covariance processing;
- updates to LEAPR for generating thermal scattering data;
- updates to PURR for unresolved resonance probability tables;
- updates to THERMR for thermal scattering data;
- integration of an NJOY2012 update file from the IAEA.

Previously, the NJOY test suite was composed of 21 tests. With this work, the test suite was expanded by adding a total of 21 new tests, for a total of 42 tests.

This report details all changes made to NJOY2016 to allow for correct processing of the ENDF/B-VIII.0 evaluated nuclear data library. All changes described here have been backported into NJOY2012 as well.

With NJOY2016, all changes to the source code are handled through pull request on the NJOY2016 git repository hosted on GITHUB which can be found here: `https://github.com/njoy/NJOY2016`. Links to relevant pull requests will be given for each change.

Chapter 2

ENDF-6 Format Changes

2.1 Tabulated Fission Energy Release Components

Evaluated data for the fission energy release components have been available in the ENDF format in section MF1/MT458 since its introduction in the ENDF-5 format in 1983. Today, the MF1/MT458 section allows an evaluator to describe these components and their energy dependence in three different ways:

- the thermal point evaluation using Sher and Beck energy dependence systematics (the original ENDF-5 format);
- the polynomial evaluation using polynomial energy dependence systematics (introduced in the ENDF-6 format in 2010);
- the tabular evaluation using tabulated energy dependence (introduced in the ENDF-6 format in 2017).

Changes were made to MODER to be able to read the new section when changing between ASCII and binary mode. The introduction of the tabulated fission energy release components also requires changes in HEATR so that these new data can be used. The implementation in the HEATR module was also changed so that all format types are used consistently. The partial fission KERMA is now calculated as:

$$k_f^n(E) = \left[Q_k(E) + Q_{\gamma,p}(E)\right] \sigma_f(E) \tag{2.1}$$

for all evaluation types. Q_k is the kinetic energy of the fission products and $Q_{\gamma,p}$ is the prompt gamma contribution. For evaluations using a polynomial representation Equation 2.1 was already used, but for evaluations using thermal point the following formula was used instead:

$$k_f^n(E) = \left[Q_{ENDF} - Q_{\gamma,d}(0) - Q_\beta(0) - \delta Q_{n,p}(E) - \bar{\nu}_t(E)\,\overline{E}(E)\right] \sigma_f(E) \tag{2.2}$$

in which Q_{ENDF} is fission Q value from MF3/MT18, $Q_{\gamma,d}(0)$ and $Q_\beta(0)$ are given in MF1/MT458, $\delta Q_{n,p}(E)$ is an analytic function defined for the thermal point evaluation, $\bar{\nu}_t$ is the total number of neutrons and $\overline{E}$ is the average fission neutron energy.

As a result, evaluations using thermal point will now give slightly different heating values because the implementation in HEATR now uses Equation 2.1 instead (differences of the order of 0.1 % can

be observed for most energies, at energies above 10 MeV this can be quite higher). The polynomial type still yields the same values (the implementation has changed somewhat but the actual formula that is used was not). For more information on these changes and the impact on the fission heating, we refer to reference [3].

Because of changes in the HEATR implementation for the thermal evaluation, test 7 and test 19 have been updated because of changes in the results. Test 24 and 26 were added to the test suite to respectively test the new tabulated fission energy release components and the case when no MF1/MT458 is given.

Links: Pull request 34, Pull request 54, Pull request 56, Pull request 58, Pull request 66

2.2 Sub-actinide Fission

Fission cross sections can now be given in MF10/MT18, if the projectile is not a neutron or if the target is not an actinide. This avoids specifying all mandatory information in an ENDF-6 file, like fission resonance widths, average number of fission neutrons, prompt fission neutron spectrum, etc. which is used in the normal case of a neutron and an actinide.

Changes were made to GROUPR so that the new MF10/MT18 section is used properly when doing automated processing. To specifically request the processing of the MF10/MT18 section in GROUPR, the mfd number 40,000,000 can now be used.

Links: Pull request 55

2.3 Fission Neutron and Gamma Emission Probabilities

The ENDF-6 format now allows an evaluator to store fission neutron and gamma emission probabilities $P(\nu, E)$ in the MF6/MT458 section. The probability $P(\nu, E)$ is the probability of a fission event accompanied by ν prompt neutrons/gammas as a function of the incident energy E. The actual data that is actually stored in MF6/MT18 is $\hat{P}(\nu, E) = P(\nu, E)/\overline{\nu}(E)$ but this has no effect on the actual structure of the new section.

Changes were made to MODER to be able to read the new section when changing between ASCII and binary mode, as well as changes to GROUPR and ACER to make sure the data is properly skipped as no output formats are currently available to be able to use these emission probabilities.

It should be noted that this format has evolved significantly since its initial inclusion in the ENDF-6 format. As a result, NJOY had to be changed multiple times to accommodate the changing format specification.

Links: Pull request 33, Pull request 35, Pull request 42

Chapter 3

Other Updates and Fixes

3.1 ACE File Plotting in ACER

Test 24 in the NJOY test suite was added to test changes in HEATR due to the introduction of tabulated fission energy release components (see section 2.1 for more information). The test uses ENDF/B-VIII.0b7 ^{239}Pu with which ACER had problems when producing the plot file (a floating point exception occurred or a NaN was produced depending on the build type). The problem was traced back to the secondary neutron energy and angular distribution for MT37 (n,4n) in the evaluation. The floating point exception or NaN occurred due to the lack of data in a hardcoded incident energy range so the z range of the plot was evaluated as going from zero to zero. When generating the plot data for VIEWR, ACER takes the logarithm of the z range, which in this case means calculating log(0) as the z-axis uses a logarithmic scale. A test was added to avoid having a z range going from zero to zero. A similar issue occurred when plotting thermal scattering data for ENDF/B-VIII.0 H-ZrH.

Another change made to ACER related to plotting was to provide proper initialisation of the ACE file title to avoid a crash in VIEWR if the user did not wish to change the title from the ACE file he wished to check in the second ACER run.

Links: Pull request 59, Pull request 67, Pull request 68

3.2 Formatting Thermal Scattering Data in ACER

Under certain conditions, ACER can produce cosine values outside of the -1,+1 range. Dan Roubtsov (CNL, Canada) proposed a number of changes to eliminate this problem.

Test 25 was added to the NJOY test suite to test the formatting of the thermal scattering data in ACER (each weight option is tested).

Links: Pull request 56, Pull request 66

3.3 Covariance Processing in ERRORR

When processing the cross section covariances of an ENDF/B-VIII.0 beta evaluation of ^{40}Ca, the ERRORR module of NJOY appeared to enter an infinite loop. ^{40}Ca is an LRF=7 resonance evaluation and includes an MF32 resonance covariance file. As a result, ERRORR uses its built-in Sammy routines to calculate the derivative of the resonances in the processing of the covariance data. In the case of ^{40}Ca, the algorithm used to calculate these derivatives breaks down at around 768 keV due to an extremely steep increase of the (n,p) cross section. The algorithm works this way: it will calculate the cross section from the resonance parameters at an energy e and then evaluate a convergence criterion. If it fails, it will try again using the average of the last successful energy value *eel* and this energy e. Due to the steep increase the value of e will get closer and closer to *eel* until it is numerically equal to *eel*. When this happens, the convergence criterion is automatically satisfied because the cross section values at *eel* and e are the same (since $e = eel$). When this happens, the algorithm will set *eel* to be equal to e to start with the next energy point. However, e is equal to *eel* so the algorithm continues to try to advance beyond the same energy point over and over again.

By adding an additional test so that the convergence criterion is tested only when *eel* remains smaller than e we can avoid the issue. To alert the user of the issue, a warning message has been added when this happens. When e is equal to *eel*, the convergence criterion is not tested and the algorithm will continue as if it were converged normally.

A cosmetic correction was also made to ERRORR so that the correct energy range is printed to the output file when processing an MF35 file (previously, the energy values of the last covariance range were printed regardless of which range was being used). Test 27 was added to the NJOY test suite as a result of this change to complement some of the ERRORR tests already present in the test suite.

Other changes were made to ERRORR to fix a crash when it tries to read over the end of the ENDF file when looking for a specific temperature and to fix a crash when using a binary GENDF file. Test 34 was added to the test suite to detect this issue in the future.

Links: Pull request 60, Pull request 68, Pull request 81

3.4 Generating Thermal Scattering Data in LEAPR

During the development of ENDF/B-VIII.0, Ignacio Marquez Damian (CAB, Argentina) and others shared both their ENDF thermal scattering evaluations as well as the LEAPR inputs they used to generate them. Ignacio Marquez Damian shared two fixes to LEAPR to overcome problems with some of these LEAPR input files, one fix for inputs involving molecules using secondary scatterers (such as SiO2) and another one to fix issues when processing ortho-H, para-H, ortho-D and para-D. Two NJOY inputs were added to the test suite (test 22 and 23) to detect these problems in the future.

Ignacio Marquez Damian also made another correction to LEAPR involving an issue with a global and local variable with the same name so that the input for H2O and D2O that were used to generate the thermal scattering files in ENDF/B-VIII.0 run correctly in NJOY 2016 (the production work was actually performed using NJOY 2012 and not NJOY 2016). Test 33 was added as a result of this change.

Links: Pull request 19, Pull request 78

3.5 Probability Table Calculation in PURR

Three bug fixes were made in PURR following ENDF/B-VIII.0 processing issues.

The first fix relates to heating values included in the probability tables. If a user asks for partial heating values for MT302 and MT402 but not MT318 in HEATR (which seems reasonable if the isotope in question is not fissionable), PURR will then try to use the partial heating values to account for fluctuations in the heating values when generating probability tables. However, the fact that MT318 is missing means that the heating values for it were never set. The array that is used to store these values was never initialised, so the uninitialised values were then used when PURR calculates the final heating values to be put in the probability table. Depending on the compiler and build type used, this may lead to an NaN value to be propagated to the output file or a floating point exception somewhere down the line. This problem goes away when properly initialising the array for the heating values.

The second fix aims to eliminate bins with zero probability when generating the probability table. Some time ago, Paul Romano (ANL) proposed a fix to PURR to correct a division by zero he observed for ^{210}Po from ENDF/B-VIII.0b7. The fix by itself was straight forward and has been implemented (even though it should no longer occur). However, when investigating the reason behind the division by zero, it became clear that the probability table was inherently wrong for ^{210}Po.

The way PURR works is that it will generate a number of samples of cross section values corresponding to randomly sampled energy values over a predetermined energy range. This energy range is determined using (among other things) the lowest value of the average level spacing defined for the unresolved resonance parameters. It is here that things went wrong. To find this value, NJOY first initialises the minimum value to 500 eV after which it compares with the available data from the evaluation. If it is lower than the previous minimum value, NJOY sets the minimum value to the new value until all values have been tested. For ^{210}Po, the minimum value remained 500 eV because the lowest value for the average level spacing was around 30 keV. This resulted in a negative value for the number of resonances and the upper energy limit becoming negative while the lower energy limit remained positive (these last two values determine the energy range).

The resulting energy value sampling led to the generation of cross section values of which 9500 were exactly the same (PURR samples 10,000 cross section values). When constructing the probability bin limits, NJOY thus ran out of different cross section values to generate these bin limits. Due to the logic by which this is done in NJOY, it lead to the generation of bin limits that were actually smaller than the previous limit. As a result, no samples were accumulated in this bin and any following bins, giving a zero probability and zero cross section value. This zero cross section value then caused the division by zero when processing ^{210}Po from ENDF/B-VIII.0b7. This problem does not occur for nuclides with an average level spacing of less than 500. For example, for ^{235}U, this is 0.7 eV.

This issue was corrected, and NJOY will now signal this exact problem should it occur again in the future. In addition, PURR will now signal the presence of remaining zero probability bins and occurrences of negative cross section values.

No test was added to the test suite because the issue already occurred in test 21 using ^{58}Fe from ENDF/B-VIII.0b4: ^{58}Fe has a minimum level spacing of 6025 eV but it did not lead to a division by zero as with ^{210}Po so the issue went undetected.

The third fix was made following the appearance of negative cross section values in the probability

table for ^{240}Pu. This is not a really a bug fix, as the problem was traced back to an error in the ^{240}Pu evaluation. In all known cases up to this one, negative cross section values in the probability table appear because the evaluation has an LSSF flag of 0 (MF3 contains background cross sections) and those background cross sections in the unresolved resonance region are negative (an example of this behaviour would be ^{22}Na, ^{36}Ar and ^{106}Cd which are the only nuclides in ENDF/B-VIII.0 to have this problem). However, for ^{240}Pu, the evaluation does not use background cross sections because LSSF is set to 1 (MF3 contains the actual dilute cross sections and the unresolved resonance parameters should only be used for self-shielding purposes). It appeared that the total cross section in the ^{240}Pu evaluation is smaller than the elastic scattering cross section in the beginning of the unresolved energy range. For example, at 5.7 keV, the total and elastic scattering cross sections are respectively 14.19534 and 15.271 barns.

The negative cross sections in the probability tables appear because PURR uses the difference of the total with elastic, fission and capture as a background/competitive cross section for the total cross section in the probability table if the LSSF flag is set to 1. In the case of ^{240}Pu, this became a negative value because the total is smaller than elastic, leading to negative cross sections in the first few bins of the probability tables. For the cross sections coming out of RECONR, NJOY actually recalculates the total cross section from the partials so this should not be an issue anywhere else.

This was not the only issue with ^{240}Pu. In the upper part of the unresolved resonance region, the total cross section also appeared to be larger than the sum of its components. Because the probability tables produced by PURR only handle 4 reactions (total, elastic, fission and capture), it is still possible to have a total cross section larger than the sum of its components but only if there is an inelastic and/or absorption competition reaction present in the unresolved energy region and then only above the competition threshold. For the ENDF/B-VIII.0 ^{240}Pu evaluation, there is no competitive reaction present. As a result, NJOY thus incorrectly assigned a positive total background in the upper part of the unresolved resonance region.

This issue was corrected as follows. When LSSF=1, the total background will be set to 0 in the following cases:

- the total cross section is smaller than the sum of its components;
- the total cross section is larger than the sum of its components when there is no competition;
- the total cross section is larger than the sum of its components below the competition threshold when there is a competitive reaction (inelastic and/or absorption).

In addition, PURR will also issue a message to indicate this has happened and at which energy so that the evaluation may be fixed.

However, it also became clear that NJOY only tested competition up to MT102 (neutron capture) and omitted checking reactions like MT5 (n,anything), MT103 (n,p) or MT107 (n,a). As a result, for some nuclides NJOY did not capture the competition flags properly, leading MCNP or other codes using the probability tables to potentially calculate the total cross section in the unresolved resonance region incorrectly (MCNP recalculates the total cross section from the values of the other 3 reactions in the probability table taking into account the possible competition reactions indicated by the flags). In most cases, the impact of this error is assumed to be small as the reactions with an MT number above MT102 are generally quite small. However, there may be nuclides for which this is not true but none have been detected so far.

Tests 10, 19 and 21 were updated following these changes. Test 31 was added to the test suite to detect total cross section issues with LSSF=1 similar to the ones encountered with ^{240}Pu in the future. Tests 35 to 42 were added to test the inelastic and absorption competition flags determined by PURR and used in ACER to be included in ACE files. These 8 additional tests cover all possible combinations of the competition flags (no competition, only inelastic competition, only absorption competition and both) for each possible value of the LSSF flag (0 or 1).

Additional updates will be made to PURR related to this issue: proper checking of competition reactions to determine if a positive difference between the total cross section and the elastic, fission and capture cross section is due to actual competition or a possible error of the total; properly setting the inelastic and absorption competition flags, etc.

Links: Pull request 18, Pull request 59, Pull request 73, Pull request 83

3.6 Processing Thermal Scattering Data in THERMR

Two bug fixes were made in THERMR following ENDF/B-VIII.0 processing issues.

The first fix is related to free thermal gas scattering. When processing thermal scattering data using the free thermal gas model, the THERMR module uses a hardcoded beta grid (this determines the energy transfer in a scattering event). Prior to these changes, this grid contained 9 values with a maximum value of 25. This has been the default for many years but when processing some nuclides at low temperatures, THERMR can fail because this grid is insufficiently large - especially when using an upper limit of 10 eV for the incident energy. This happened twice when processing ENDF/B-VIII.0 beta libraries, first for ^{56}Fe (the grid was then expanded to 400 for a total of 30 values) and another time for H1 (the grid was expanded up to 3500 with an additional 15 values).

The results for test 1 of the NJOY test suite were impacted by this change, but only for the first beta grid expansion. Differences were observed for the highest two incident energies (1.16 and 1.28 eV) and the lower outgoing energies (below .5 eV) so the changes appear only for the larger values of the energy transfer (larger beta values). The lower outgoing energies up to 0.5 eV are different and the associated cosines are slightly different, but not by much. The cosines differ at the third or fourth digit after the decimal point (e.g. -0.990690 vs -0.990396). The second expansion of the beta grid did not influence this test as the added beta values were too large for the energy transfer that is possible in the nuclide used for test 1.

The second fix is related to formatting the thermal scattering data (both for free thermal gas scattering and $S(\alpha, \beta)$ data). THERMR allows a user to chose two formats, the original ordering E, E', μ that was already available in NJOY99 (iform=0, referred to as the MF6 special format) and the new ordering E, μ, E' that was added to NJOY2012 (iform=1, referred to as the MF6 law7 format). When using this second format, THERMR crashed when processing Zr in ZrH thermal scattering data at 296 K (reported by C. Mattoon, LLNL). This was traced back to a division by zero when performing Lagrangian interpolation on the incoherent inelastic scattering cross sections because the incident energy array was not initialised properly for this format.

Test 32 (which processes thermal scattering data in both formats) was added to the test suite to detect this issue in the future.

Links: Pull request 66, Pull request 67, Pull request 74

3.7 Integration of the IAEA NJOY2012 Update File

Daniel Lopez-Aldama (NDS, IAEA) provided his NJOY2012 update file for integration into NJOY2016. Similar update files provided by other users will be integrated into NJOY2016 when these changes are deemed relevant for the global user community on a case by case basis.

The integration of this NJOY update file lead to changes in ACER, GROUPR and PURR.

NJOY2016 and its predecessor NJOY2012 have a hardcoded option that smooth centre-of-mass energy distributions from MF6 and histogram energy distributions for delayed neutrons at lower energy using a $\sqrt{E}$ shape, and to add additional points above 10 Mev to some fission spectra assuming an exponential shape. To change the setting of this option, NJOY has to be recompiled. ACER and GROUPR were modified so that this option can be changed in the input file, thus not requiring a user to recompile NJOY when he wished to change this option. Tests 28 and 29 were added to the NJOY test suite to track these new input options for ACER and GROUPR.

Additional changes were made to ACER and GROUPR to correct an issue when using Kalbach-Mann systematics for describing energy and angular distributions for secondary particles in MF6.

PURR was corrected to properly set the MT number for the absorption competition in a probability table. Previously, NJOY incorrectly set this value to the elastic competition MT number.

The update file also contained a change for MATXSR when formatting the MATXS output file. The issue that this change referred to could not be reproduced so it was decided not to add it to NJOY2016. An additional test (test 30) was however added to the NJOY2016 test suite to complement MATXSR testing already present in the test suite.

Links: Pull request 69

References

[1] D. A. Brown et al., "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data", *Nucl. Data Sheets*, **148** (2018)

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[3] W. Haeck, "New fission heating capabilities in the NJOY2016 HEATR module", LANL Report LA-UR-18-22546